

# Pairing mechanism for high temperature superconductivity in the cuprates: what can we learn from the two-dimensional $t - J$ model?

Huan-Qiang Zhou<sup>1</sup>

<sup>1</sup>Centre for Modern Physics and Department of Physics,  
Chongqing University, Chongqing 400044, The People's Republic of China

More than twenty years have passed since high temperature superconductivity in the copper oxides (cuprates) was discovered by J.G. Bednorz and K.A. Müller in 1986 [1]. Although intense theoretical and experimental efforts have been devoted to the investigation of this fascinating class of materials, the pairing mechanism responsible for unprecedented high transition temperatures  $T_c$  remains elusive. Theoretically, the difficulty lies in the fact that this class of materials, as doped Mott-Hubbard insulators [2], involve strong electronic correlations, which renders conventional theoretical approaches unreliable. Recent progress in numerical simulations of strongly correlated electron systems in the context of tensor network representations [3, 4] makes it possible to get access to information encoded in the ground-state wave functions of the two-dimensional  $t - J$  model—a minimal model, as widely believed, to understand electronic properties of doped Mott-Hubbard insulators [5–8]. In this regard, an intriguing question is whether or not the two-dimensional  $t - J$  model holds the key to understanding high temperature superconductivity in the cuprates. As it turns out, such a key lies in a superconducting state with mixed spin-singlet  $d + s$ -wave and spin-triplet  $p_x(p_y)$ -wave symmetries in the presence of an anti-ferromagnetic background [9]. Here, the  $d + s$ -wave component in the spin-singlet channel breaks  $U(1)$  symmetry in the charge sector, whereas both the anti-ferromagnetic order and the spin-triplet  $p_x(p_y)$ -wave component breaks  $SU(2)$  symmetry in the spin sector. Therefore, four gapless Goldstone modes occur. However, even if we resort to the Kosterlitz-Thouless transition [10], *only* the  $d + s$ -wave superconducting component survives thermal fluctuations. This turns three gapless Goldstone modes, arising from  $SU(2)$  symmetry breaking, into two degenerate soft modes, with twice the spin-triplet  $p_x(p_y)$ -wave superconducting energy gap as their characteristic energy scale: one is a spin-triplet mode observed as a spin resonance mode in inelastic neutron scattering, the other is a spin-singlet mode observed as a  $A_{1g}$  peak in electronic Raman scattering. The scenario allows us to predict that pairing is of  $d + s$ -wave symmetry, with the two degenerate soft modes as the long-sought key ingredients in determining the transition temperature  $T_c$ , thus offering a possible way to resolve the controversy regarding the elusive mechanism for high temperature superconductivity in the cuprates.

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Imagine if we would have been able to solve a model system describing doped Mott-Hubbard insulators on a two-dimensional square lattice, whose ground-state wave function is a superconducting state with mixed spin-singlet  $d + s$ -wave and spin-triplet  $p_x(p_y)$ -wave symmetries in the presence of an anti-ferromagnetic background, with the order parameters for the  $s$ -wave,  $d$ -wave, and  $p_x(p_y)$ -wave superconducting components, together with the anti-ferromagnetic order parameter, shown in Fig. 1, in a proper doping range. Note that  $\Delta_d$  and  $\Delta_s$  are, respectively, the spin-singlet  $d$ -wave and  $s$ -wave superconducting energy gaps, whereas  $\Delta_p$  is the spin-triplet  $p_x(p_y)$ -wave superconducting energy gap and  $N$  is the anti-ferromagnetic Néel order parameter. A few peculiar features of this state are: (i) Both the 90 degree (four-fold) rotation symmetry and the translation symmetry under one-site shifts are spontaneously broken on the square lattice. (ii) Spin-rotation symmetry  $SU(2)$  is spontaneously broken, due to the simultaneous occurrence of both the  $p_x(p_y)$ -wave superconducting component and the anti-ferromagnetic order. (iii)  $U(1)$  symmetry in the charge sector is spontaneously broken, due to pairing in both spin-singlet and spin-triplet channels. Here, we emphasize that the symmetry mixing of the spin-singlet and spin-triplet channels arises from the spin-rotation symmetry breaking, *simply because spin is not a good quantum number*. (iv) All superconducting components are homogeneous, in the sense that their superconducting order param-

eters are independent of sites on the lattice.

Now let us switch on thermal fluctuations. Suppose we restrict ourselves to a strict two dimensional system. Then, even if the Kosterlitz-Thouless transition [10] is invoked, *only* spin-singlet  $d + s$ -wave superconducting component survives thermal fluctuations. However, the non-abelian  $SU(2)$  symmetry is not allowed to be broken at any finite temperature [11, 12]. This immediately implies that the Goldstone modes arising from the spontaneous symmetry breaking of  $SU(2)$  in the spin sector have to be turned into degenerate soft modes, with twice the spin-triplet  $p_x(p_y)$ -wave superconducting energy gap as their characteristic energy scale: one is a spin-triplet mode associated with the anti-ferromagnetic order, with the momentum transfer  $(\pi, \pi)$ , and the other is a spin-singlet mode associated with the spin-triplet  $p_x(p_y)$ -wave superconducting component, with the momentum transfer  $(0, 0)$ . On the other hand, there is nothing to prevent from the breaking of the discrete four-fold rotation symmetry on the square lattice. Actually, this broken symmetry not only manifests itself in the admixture of a small  $s$ -wave component to the dominant  $d$ -wave superconducting state (see Fig. 1, left panel), but also protects the spin-singlet soft mode that is unidirectional as it arises from the  $p_x(p_y)$ -wave superconducting component.

Our argument leads to a scenario that, at any finite temperature, the pairing is of  $d + s$ -wave symmetry, with two degenerate soft modes acting as the key ingredients in deter-

mining the transition temperature  $T_c$ . Actually, two distinct energy scales  $2\Delta^*$  and  $E_{\text{res}}$  are involved, in a marked contrast with the conventional superconductors:  $2\Delta^*$  arises from the anti-ferromagnetic Néel order parameter  $N$ , which is responsible for pairing, with its coupling strength decreasing almost linearly with doping, whereas  $E_{\text{res}} = 2\Delta_p$ , which is responsible for condensation. Therefore,  $E_{\text{res}}$  must scale with the superconducting transition temperature  $T_c$ , i.e.,  $E_{\text{res}} \sim k_B T_c$ , with  $k_B$  being the Boltzmann constant [see Fig. 1, right panel]. Similarly,  $2\Delta^*$  scales as  $2\Delta^* \sim k_B T^*$ , with  $T^*$  being the so-called pseudogap temperature [13, 14]. In addition, one may expect that  $E_{\text{res}} < 2\Delta_d$ , simply due to the fact that the predominant  $d$ -wave superconducting component survives thermal fluctuations. Considering that both the superconducting gap  $\Delta_d$  and the transition temperature  $T_c$  characterize the superconductivity, they should track each other in the entire doping range, implying  $\Delta_d \sim k_B T_c$ . In fact, for the  $t-J$  model, our simulation indicates that  $E_{\text{res}} \approx 1.25\Delta_d$  [9]. This in turn allows us to estimate a universal coefficient  $\kappa \approx 5.37$  in the scaling relation:  $E_{\text{res}} = \kappa k_B T_c$ .

Note that the two distinct energy scales in the underdoped regime are split off from one single energy scale in the (heavily) overdoped regime. This naturally results in a crossover from the Bose-Einstein condensation (BEC) regime to the Bardeen-Cooper-Schrieffer (BCS) regime, as conjectured in Ref. [15], which in turn is essentially equivalent to the phase fluctuation picture proposed by Emery and Kivelson [16]. However, there is an important difference: the superconductivity weakens in the heavily underdoped regime, not only because of the loss of phase coherence, but also because of the decrease of the superconducting gap  $\Delta_d$  with underdoping.

Now a fundamental question is whether or not such a scenario is really relevant to the high  $T_c$  problem. This brings us to the phenomenology of the high temperature cuprate superconductors.

First, let us focus on the two distinct energy scales  $2\Delta^*$  and  $E_{\text{res}}$ . Physically, the two distinct energy scales measure, respectively, the pairing strength and the coherence of the superfluid condensate. This naturally leads to two different phases: one is characterized by incoherent pairing, which may be identified with the pseudogap phase; the other is associated with the emergence of a coherent condensate of superconducting pairs, which may be identified with the superconducting phase of  $d+s$ -wave symmetry [see Fig. 2]. Evidence for the two distinct energy scales was reported in angle-resolved photoemission spectra [17–20], electronic Raman spectra [21–24], scanning tunneling microscopy [25],  $c$ -axis conductivity [26], Andreev reflection [27], magnetic penetration depth [28], and other probes (for a review, see, Ref. [29]). Actually, these studies indicate that the gap near the antinodal region, which is identified as the pseudogap, does not scale with  $T_c$  in the underdoped regime, whereas the gap near the nodal region may be identified as the superconducting order parameter in the cuprates [17–23]. This identification offers a natural explanation why the two distinct energy scales in the underdoped regime merge into one single energy scale in the

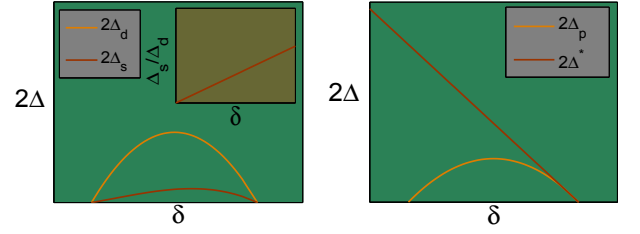


FIG. 1: (color online) The doping dependence of the order parameters for a model system describing doped Mott-Hubbard insulators on a two-dimensional square lattice, whose ground-state wave function is a superconducting state with mixed spin-singlet  $d+s$ -wave and spin-triplet  $p_x(p_y)$ -wave symmetries in the presence of an anti-ferromagnetic background, with the order parameters for the  $s$ -wave,  $d$ -wave, and  $p_x(p_y)$ -wave superconducting components, together with the anti-ferromagnetic order parameter  $N$ . Left panel: The superconducting gaps  $\Delta_d$  and  $\Delta_s$  for the spin-singlet  $d$ -wave and  $s$ -wave components as a function of doping  $\delta$ , with their ratio  $\Delta_s/\Delta_d$  shown in the inset. Right panel: The energy scales  $2\Delta^* \sim k_B T^* \sim N$  and  $E_{\text{res}} = 2\Delta_p$  for the anti-ferromagnetic order and the spin-triplet  $p_x(p_y)$ -wave superconducting order as a function of doping  $\delta$ , with  $N$  being the anti-ferromagnetic order, and  $k_B$  the Boltzmann constant. A crossover from the Bose-Einstein condensation (BEC) regime to the Bardeen-Cooper-Schrieffer (BCS) regime occurs, when the two energy scales merge into one single energy scale in the (heavily) overdoped regime. Note that, in general,  $E_{\text{res}} < 2\Delta_d$ . Indeed,  $E_{\text{res}} \approx 1.25\Delta_d$ , as predicted from the two-dimensional  $t-J$  model. In addition,  $E_{\text{res}}$  scales with the superconducting transition temperature  $T_c$ :  $E_{\text{res}} \sim k_B T_c$ .

(heavily) overdoped regime as a consequence of the evolution of the Fermi arcs in the underdoped regime to a large Fermi surface in the (heavily) overdoped regime [30, 31]. We emphasize that the pseudogap near the antinodal region does not characterize a precursor to the superconducting state, in the sense that the pseudogap smoothly evolves into the superconducting gap at  $T_c$  [13, 30, 31]. Instead, it coexists with the superconducting gap of the  $d+s$ -wave symmetry in the superconducting state. More likely, a precursor pairing occurs in the nodal region [32], with its onset temperature lower than  $T^*$ , but above  $T_c$ , which may be identified with the Nernst regime [33, 34]. As observed, the superconducting gap near the nodes scales as  $k_B T_c$  [29]. This makes a strong case for our argument, if one takes into account the smallness of the  $s$ -wave superconducting gap. On the other hand, ample evidence has been accumulated, over the years, for the universal scaling relation  $E_{\text{res}} = \kappa k_B T_c$ , valid for both soft modes, i.e., the spin-triplet resonance mode in inelastic neutron scattering experiments [35–41] and the spin-singlet mode observed as a  $A_{1g}$  peak in electronic Raman scattering [21, 42–46], respectively. The experimentally determined  $\kappa$  is around 6, quite close to our theoretical estimate. This presents a possible resolution to the mysterious  $A_{1g}$  problem [42]: the  $A_{1g}$  mode is a charge collective mode as a bound state of (quasiparticle) singlet pairs originating from the fluctuating  $p_x(p_y)$ -wave superconducting order.

Second, is the pairing symmetry really of  $d+s$ -wave na-

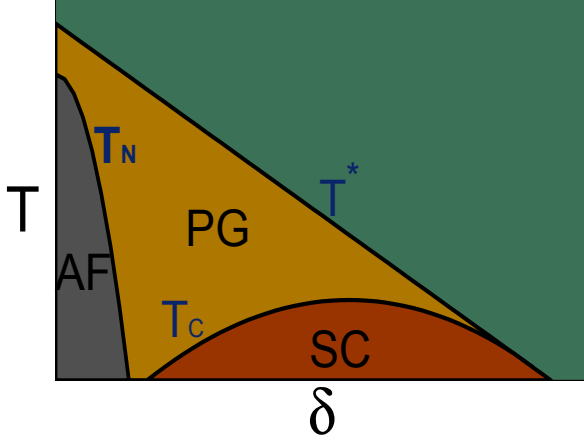


FIG. 2: (color online) A schematic phase diagram of the hole-doped high temperature cuprate superconductors plotted as a function of temperature  $T$  and hole doping  $\delta$ . Here, SC, PG, and AF stand for the superconducting, pseudogap, and anti-ferromagnetic phases, respectively.  $T_c$ ,  $T^*$ , and  $T_N$  represent, respectively, the superconducting transition temperature, the pseudogap temperature, and the anti-ferromagnetic Néel temperature. In our scenario, the PG phase is characterized by incoherent preformed pairs, with a pseudogap opening near the anti-nodal region, leaving the remnant gapless Fermi arcs near the nodes in the momentum space. In addition, the four-fold rotation symmetry and the translation symmetry are broken on the square lattice. Superconductivity occurs, when long range phase coherence develops at  $T_c$ .

ture? Many theoretical proposals, mainly based on the resonating valence bond scenario [2], predicted a pure  $d$ -wave superconductivity in the cuprates [6, 47–49]. Although a variety of experiments have demonstrated a predominant  $d$ -wave gap [50–52], strong evidence points to an admixture of an  $s$ -wave component to the dominant  $d$ -wave superconductivity in muon spin rotation studies [53, 54], electronic Raman measurements [55], angle-resolved electron tunneling experiments [56], and neutron crystal-field spectroscopy experiments [57]. In addition, a universal scaling relation of the superfluid density,  $\rho_s(0)$ , at absolute zero, with the product of the dc conductivity  $\sigma_{dc}(T_c)$ , measured at  $T_c$ , and the transition temperature  $T_c$ , indicates that a pure  $d$ -wave superconductivity is realized in the cuprates [58]. This scaling relation may be regarded as a modified form of the Uemura relation between the superfluid density  $\rho_s(0)$  and the transition temperature  $T_c$  [59, 60], which works reasonably well in the underdoped regime. However, a significant deviation from the scaling relation was subsequently observed [61], with a salient feature that the deviation increases with doping. This feature strongly suggests that the discrepancy should be accounted for by removing an extra contribution from the  $s$ -wave component in the context of the  $d + s$ -wave pairing symmetry. This issue has been addressed recently [62], thus supporting our scenario.

Third, any theory regarding the underlying mechanism of high temperature superconductivity would not be complete,

if the stripe states (for reviews, see, e.g., Ref. [63–66]) were not touched upon. Surprisingly, a stripe-like state, i.e., a state with charge and spin density wave order, coexisting with a spin-triplet  $p_x(p_y)$ -wave superconducting state, does occur as a ground state in the  $t - J$  model for dopings up to  $\delta \approx 0.18$  [9], with  $J/t = 0.4$ . Again, all symmetries, including the four-fold rotation and translation lattice symmetry,  $SU(2)$  spin rotation and  $U(1)$  charge symmetry, are spontaneously broken. A similar line of reasoning yields that, *only* the charge density wave order survives thermal fluctuations, with the concomitant occurrence of the soft modes: they arise from the  $SU(2)$  symmetry breaking of the spin density wave order and the spin-triplet  $p_x(p_y)$ -wave superconducting order, with twice the spin-triplet  $p_x(p_y)$ -wave superconducting energy gap as their characteristic energy scale. Although it remains uncertain whether or not such a commensurate stripe-like state is an artifact of our choice of the unit cell for the tensor network representation of quantum states, an important lesson we have learned from our simulation is that, the  $t - J$  model exhibits a strong tendency towards a stripe state in the underdoped regime, consistent with the density matrix renormalization group [67] for a more realistic stripe pattern at doping  $1/8$  and  $J/t = 0.35$ . From this we conclude that (i) static charge density wave order is compatible with the superconductivity, so its possible role is deserved to be explored in the formation of the pseudogap; (ii) static spin density wave order is detrimental to the  $d + s$ -wave superconductivity, because no  $d + s$ -wave superconducting component coexists with the charge and spin density order in the ground state; (iii) fluctuating spin density wave order, together with the fluctuating spin-triplet  $p_x(p_y)$ -wave superconducting order, equally well account for the Bose-Einstein condensation in our scenario. Therefore, the fluctuating stripe order is intrinsic to many, if not all, families of the high temperature cuprate superconductors.

Fourth, does our prediction about the spontaneous breaking of the four-fold rotation symmetry and the translation symmetry under one-site shifts in the pseudogap phase represent a physical reality? In our scenario, the PG phase is characterized by incoherent preformed pairs, which occur in the anti-nodal regime in the momentum space, leaving the remnant gapless Fermi arcs in the nodal regime. In addition, the four-fold rotation symmetry and the translation symmetry are broken on the square lattice. In the superconducting phase, the four-fold rotation symmetry breaking manifests itself in the admixture of an  $s$ -wave component to the dominant  $d$ -wave state. In the pseudo phase, the broken symmetry protects the spin-singlet soft mode that is unidirectional as it arises from the  $p_x(p_y)$ -wave superconducting fluctuations, as well as the fluctuating spin density order and possibly static charge density order. One may expect that measurable physical effects arise from the coupling of electrons with the unidirectional spin-singlet soft mode. Indeed, a large in-plane anisotropy of the Nernst effect in  $\text{YBa}_2\text{Cu}_3\text{O}_y$  was reported that sets in exactly at the pseudogap temperature  $T^*$  [68]. This broken four-fold rotation symmetry was also detected by resistivity [69]

and inelastic neutron scattering [70–72] at low doping, and by scanning tunneling spectroscopy [73, 74] at low temperature, without a clear connection to the pseudogap temperature  $T^*$ .

Fifth, what is the real bosonic glue for high temperature superconductivity in the cuprates? Many researchers have suggested various candidates, such as the spin resonance mode [75, 76], the spin fluctuation spectrum [77–81], the phonon spectrum [82, 83], a mode responsible for the dip observed in angle-resolved photoemission spectra [84], and the anti-ferromagnetic fluctuations [85, 86], as a possible bosonic glue. However, our scenario unveils that the spin resonance and the Raman  $A_{1g}$  modes play an analogous role to a roton in the superfluid  $^4\text{He}$ , in contrast to the conventional low-temperature superconductors with phonon-mediated pairing. This strongly suggests that, there is no bosonic glue to pair electrons in the cuprates, as advocated by Anderson [87]. That is, pairing is an emergent phenomena; it is resulted from the many-body correlations in a doped Mott-Hubbard insulator: both the  $d$ -wave and the extended  $s$ -wave pairings are realized to avoid strong on-site Coulomb repulsion. Here, we remark that the spin resonance and the Raman  $A_{1g}$  modes have been suggested by Uemura [88] to be roton analogues, by invoking soft modes in the spin and charge channels in an incommensurate stripe state (see also Ref. [89] for an alternative explanation). In this sense, our scenario unlocks the secret of the yet-to-be-achieved solid, as an analogue of the solid  $^4\text{He}$ , in the cuprates.

In closing, let us discuss a possible candidate of the model system that is able to reproduce all the features needed to address the high  $T_c$  problem, as mentioned at the beginning of the text. With the fact in mind that the two-dimensional  $t - J$  model does exhibit a  $d + s$ -wave superconducting state and a stripe-like state in a certain doping range for a physically realistic parameter regime [9], we speculate that, most likely, an extension of the  $t - J$  model to include the next-nearest-neighbor and the third-nearest-neighbor hopping terms, which are known to be significant in the cuprates, will do the job.

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